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Since Damkohler and Reynolds numbers over the range of conditions relevant to supersonic hydrogen-air combustion were found to be consistent with the combustion occurring in the reaction-sheet regime, detailed numerical integrations were performed on the structures of counterflow hydrogen-air diffusion flames, for pressures from 0.5 to 10 atm and air temperatures from 300 K to 1200 K, at a hydrogen temperature of 300 K. The results showed extinction to occur at high enough rates of strain in most cases, but no extinction for air temperatures above about 1000 K. Reduced chemical-kinetic mechanisms were developed for simplifying the computations. The computed extinction strain rates were found to be in excellent agreement with experiments. Compressibility effects were taken into account, and the results are being worked into methods for describing turbulent combustion in high-speed flows.

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THEORIES OF TURBULENT COMBUSTION IN HIGH SPEED FLOWS

1. INTRODUCTION

Uncertainties about turbulent combustion in hydrogen-air systems have an impact on our abilities to achieve successful designs of supersonic combustion devices for the National Aerospace Plane, for example. As a step toward addressing problems in this area, a research program on theories of turbulent combustion in high-speed flows was started at the University of California San Diego in March, 1989. Prior to initiation of this research, it was not known whether the combustion was more likely to occur in reaction-sheet or distributed-reaction regimes and common practice was to assume the latter and employ laminar chemical kinetics in routines based on computational fluid mechanics. In the course of this research, estimates suggest that this is a poor procedure since the reaction-sheet regime is likely to be more prevalent than the distributed-reaction regime. Therefore, much of the research was directed towards determining regimes more firmly and developing improved methods for accounting for the chemical-kinetics of the combustion in reaction-sheet regimes.

2. RESEARCH OBJECTIVES

The objective of this research has been to improve understanding of the chemical kinetics and fluid dynamics of turbulent combustion in high-speed flows. Supersonic combustion in hydrogen-air mixtures is being addressed by theoretical approaches that distinguish between reaction-sheet and distributed-reaction regimes. The work seeks to identify effects of compressibility in turbulent combustion, methods for including compressibility in theoretical analyses, and reduced chemical-kinetic mechanisms appropriate for supersonic combustion. The results may help to enhance capabilities of reasonable computations of high-speed turbulent reacting flows.

3. ACCOMPLISHMENTS

The major accomplishments of the present work are summarized in the list of publications given below. The first four items in this list refer to studies in boron combustion, which was the subject of an AFOSR grant that preceded the

present grant. These references are included here because publication of results of this earlier work has been supported by the present grant. However, the technical content of these papers is not reviewed here because the subject is different from that currently under consideration.

3.1. Turbulent Combustion Regimes in Supersonic Combustion

At the beginning of the present project, calculations were completed of Damköhler and Reynolds numbers for the anticipated range of supersonic combustion conditions in aerospace-plane applications. Reynolds numbers based on the integral scale ranged from about 10^3 to 10^7, and Damköhler numbers based on the integral scale and the overall premixed-flame reaction time ranged from about 10 to 10^4. These Damköhler numbers are not consistent with combustion occurring in the distributed-reaction regimes, but they are consistent with the occurrence of the reaction-sheet regime. As a first step towards considering the flame structures in the reaction-sheet regime, calculations were therefore made of counterflow diffusion-flame structure and extinction for hydrogen-air systems.

3.2. Counterflow Hydrogen-Air Flame Structure

The structure and extinction of counterflow diffusion flames of hydrogen and air were investigated for pressures from 0.5 to 10 atmospheres and for initial temperatures from 300 K to 1200 K as described in items 5, 6 and 7 of the publications. These conditions span the range estimated for the application to the aerospace plane. Numerical integrations were performed for air-side strain rates from 60 s^{-1} to extinction The numerical results were compared with predictions of an asymptotic analysis that involved reduction to one-step chemistry through introduction of steady-state and partial-equilibrium approximations. Reasonable agreement was found for concentrations in the main reaction zone at low strain rates but not otherwise, thereby motivating further reduced-mechanism studies, outlined later.

The computations began with a 21-step mechanism but found 8 of the steps to be relatively unimportant, so that a 13-step mechanism (among 8 species, H_2, O_2, H, O, OH, HO_2, H_2O_2, and H_2O) was obtained. For counterflow hydrogen-air diffusion flames at normal atmospheric pressure with feed streams at room temperature these computations gave an extinction strain rate of 8140 s^{-1}, nearly

twice the best experimental value available at the time. However, the experiments involved jets that had not closely approximated the potential-flow boundary conditions of theoretical computations. Subsequently, Pellett et al. at NASA Langley (AIAA Preprint 91-0370) improved the experiment to match the boundary conditions of the theory better and obtained an extinction strain rate of 8250 s^{-1} in excellent agreement with the prediction. Additional calculations for fuels diluted with nitrogen showed agreement with experiment to remain excellent over the entire dilution range.

Since peak combustor temperatures on the order of 3000 K are anticipated for some operating conditions with hydrogen-air flames, questions arose concerning possible influences of nitrogen chemistry on flame structure and extinction. We therefore augmented our chemical-kinetic scheme to include nitrogen chemistry. Results demonstrated negligible influences of nitrogen chemistry on flame structure and extinction. The largest effect was a decrease in peak flame temperature by about 30 K when 10^{-3} ppm of NO was added to the air stream. For these developed flames nitrogen chemistry is unimportant; influences on ignition have not yet been investigated.

Simpler kinetics are desirable to enable computations to be performed in more complex configurations. The major route to simplification is provided by employing reduced chemical-kinetic mechanisms. A four-step mechanism is obtained by imposing steady states for HO_2 and H_2O_2. A three-step mechanism results from further introducing an O-atom steady state, and a two-step mechanism by further imposing the steady state for OH. Flame-structure computations have now been completed with each of these reduced mechanisms. The agreement with results of the full mechanism is good and improves with increasing strain rate, resulting in excellent extinction predictions, even for the two-step mechanism. This indicates good utility of reduced mechanisms. The two-step mechanism is the simplest, generally useful one because it is known that a one-step approximation, in which the H-atom steady state is employed as well, gives very poor extinction predictions.

3.3. Simplified Descriptions of Counterflow Flames in Turbulent Combustion

Experimental results for counterflow axial velocity as a function of axial coordinate will depend appreciably on flow configuration, as may be inferred from the literature that considers potential flow and plug-flow boundary conditions. These and other aspects of flames have been discussed in a review cited as item 8 of the publications. New theoretical analyses reported in publication 9 have applied asymptotic methods for large Reynolds and Zel'dovich numbers to predict displacement effects resulting from heat release in different counterflow configurations. It was found for methane-air flames, for example, that in a representative experiment, the air-side strain rate of 540 s^{-1} for the one-term expansion is increased to 710 s^{-1} for the two-term expansion, demonstrating the importance of the displacement correction. The composite expansion involving one-term inner and two-term outer results yields remarkably good agreement with results of full numerical integrations and of experiment.

3.4. Compressibility Effects in Various Flow Fields Related to Supersonic Combustion

Studies directed towards ascertaining influences of kinetic energy, compressibility and high Mach numbers in high-speed combustion have now addressed a variety of different flow configurations, as indicated in publications 10, 11 and 12. A theoretical analysis of the inviscid flow between a porous plate and a parallel impermeable plate was performed for small values of the ratio of the plate separation distance to the lateral extent of the plates, for both planar and axisymmetric geometries, as described in item 11 of the publications. The problem of computing the flow field was reduced to the solution of a single integral equation, which was accomplished numerically. The ratio of specific heats γ was a parameter of the solution, and parametric results were obtained from $\gamma = 1.0$ to $\gamma = 1.67$. The flow exhibited choking at a critical value of the lateral extent of the plate, in the vicinity of which the Mach number approaches unity. The results are needed in providing external boundary-layer conditions for studying the flame structure in the viscous region between two counterflowing streams when compressibility is important.

It was observed that this same general type of formulation can describe rotational compressible flow in solid-propellant rocket-motor ports, and therefore the corresponding analysis was developed in publication 12, with applications to choking in nozzleless rocket motors. These studies indicate general characteristics of compressibility effects relevant to supersonic combustion. Future work is intended to address influences of large pressure and temperature fluctuations on the combustion in high-speed flows.

It is noteworthy that these flows require subsonic injection for the analyses to be meaningful and therefore cannot be applied directly to the stagnation regions, in the moving reference frame, in the braids between vortices of a shear layer, when convective Mach numbers are supersonic. The viewpoint has been taken here that the analyses apply downstream from shocklets, where the flamelets must lie, and that in addition to the analyses of the counterflow mixing layers, descriptions must be developed of the shocklet locations in the nonpremixed supersonic combustion configurations of interest. More research therefore remains to be done on the compressibility effects in these flows.

3.5 Modeling for High Speed Turbulent Combustion

In collaboration with Professor K.N.C. Bray of Cambridge University we have been studying the special processes and mechanisms which arise in high speed turbulent combustion as distinct from those known to occur in the far better studied cases of low speed combustion. The principal differences are identified with various pressure effects and with new mechanisms of viscous dissipation. With respect to the former the current modeling of the influence of pressure fluctuations on redistributing the various contributions to the turbulent kinetic energy is the result of much research over an extended period. These models involve an integration of the velocity field over an infinite domain but when the flow is locally supersonic, the pressure at point can only depend on the flow within the upstream Mach cone and entirely new models would appear to be called for. In addition to these effects of pressure fluctuations we must expect that the mean pressure can no longer be considered thermochemically constant in high speed flows.

With respect to new dissipative processes, recent research on compressible turbulence has established that regions of sharply varying pressure, termed shocklets, although they are not well resolved in the DNS so that this terminology

may be questioned, appear to provide a new mechanism for viscous dissipation and therefore call for additional terms in the dissipation equation which is introduced in most turbulence models in order to provide length scale information. We have paid close attention to recent developments in the modeling for compressible turbulence since they have implications with respect to reacting flow.

As a result of these studies, Professor Bray, working with a graduate student, has developed a code for the study of axisymmetric turbulent combustion based on both k-ε and algebraic stress models and is in position to begin assessing the influence of new models for the pressure fluctuations and viscous dissipation. In this code a laminar flamelet description accounts for the chemical behavior.

4. PERSONNEL

The personnel who worked on this project are listed below:

		Percentage Time
Professor P.A. Libby	Principal Investigator	15%
Professor F,.A. Williams	Principal Investigator	15%
Mr. S.C. Li	Postgraduate Research Engineer	50%
Mr. G. Balakrishnan	Ph.D. Student	100%

5. PRESENTATIONS

Related talks/contributed papers by the PIs at meetings in connection with this project.are:

"Turbulent Combustion," May 1, 1989, Department of Mechanical Engineering, University of California, Santa Barbara, California.

"Asymptotic Structure and Extinction of CO/H_2 Diffusion Flames with Reduced Kinetic Mechanisms," July 24-27, 1989, Twelfth International Colloquium on Dynamics of Explosions and Reactive Systems, University of Michigan, Ann Arbor, Michigan.

"Combustion Theory - Detonations and Diffusion Flames," September 11-13, 1989, Workshop on an Introduction to Dynamical Systems, University of Minnesota, Minneapolis, Minnesota.

"Recent Advances in Theories of Structure of Diffusion Flamelets in Turbulent Combustion," October 27, 1989, Department of Mechanical Engineering, University of Colorado, Boulder, Colorado.

"Reduced Kinetic Mechanisms for Complex Combustion Chemistry," November 17, 1989, Workshop on Dynamical Issues in Combustion Theory, University of Minnesota, Minneapolis, Minnesota.

"Structures of Turbulent Diffusion Flamelets," February 14, 1990, Division of Engineering, California Institute of Technology, Pasadena, California.

"Considerations of the Structure of Premixed Hydrogen Flames," July 20, 1990, International Workshop on Flame Structure, Department of Engineering, Cambridge University, Cambridge, England.

"An Experimental and Theoretical Investigation of the Dilution, Pressure and Flow-Field Effects on the Extinction Conditions of Methane-Air-Nitrogen Diffusion Flames," "A Numerical and Asymptotic Investigation of Structurres of Hydrogen-Air Diffusion Flames at Pressures and Temperatures of High-Speed Combustion," "Vortex Modification of Diffusion Flamelets," "Ignition and Combustion of Boron in Wet and Dry Atmospheres," July 22-27, 1990, Twenty-Third International Symposium on Combustion, University of Orleans, Orleans, France.

"Do Flames Really Penetrate Vortex Cores?", July 28-29, 1990, Tenth International Workshop on Mathematics in Combustion, University of Poitiers, Poitiers, France.

"Swirl Effects on Flame Structures," seminar, November 5, 1990, Technological Institute, Northwestern University, Evanston, Illinois

"Some Advances in Combustion Theory Bearing on Fire-Safety, Energy-Production and Environmental Issues," keynote talk, March 21-22, 1990, 3rd ASME-JSME Thermal Engineering and ASME-JSME-JSES Solar Energy Conferences, Reno, Nevada.

"Turbulent Diffusion Flames," May 2, 1991, Department of Mechanical Engineering, University of Arizona, Tucson, Arizona.

"Theory of Turbulent-Jet Diffusion Flames," October 18, 1991, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

"Methods of Approximation for Calculating Structures of Real Flames," December 3, 1991, Fourth International Conference on Numerical Combustion, St. Petersburgh Beach, Florida.

"Turbulent Combustion," December 5, 1991, Department of Mechanical Engineering, University of Kentucky, Lexington, Kentucky.

6. TECHNICAL INTERACTIONS

Technical interactions included discussion with personnel in government laboratories and industry concerning aerospace-plane flight conditions and discussions with these same groups and with personnel at universities concerning results of the research. Specific people contacted are: Rocketdyne; M. Tapper; NASA Langley, T. Gatski, G. Pellett; Wright Patterson Air Force Base, M. Roquemore; University of Washington, G. Kosaly; Caltech, P. Dimotakis; University of Colorado, D. Kassoy, J. Daily.

7. INVENTIONS

There were no inventions in this project.

8. PUBLICATIONS

1. S.C. Li, "Experimental and Theoretical Studies of Ignition and Combustion of Boron Particles in Wet and Dry Atmospheres," Ph.D. Thesis, Princeton University, 1990.

2. S.C. Li, "Optical Measurement of Size Histories of Boron Particles in Ignition and Combustion States" Combustion Science and Technology 77, 149-169 (1991).

3. S.C. Li and F.A. Williams, "Ignition and Combustion of Boron in Wet and Dry Atmospheres," Twenty-Third Symposium (International) on combustion, The Combustion Institute, Pittsburgh, 1991, pp. 1147-1154.

4. S.C. Li and F.A. Williams, "Ignition and Combustion of Boron Particles," Second International Symposium on Special Topics in Chemical Propulsion: Combustion of Boron-Based Solid Propellants and Solid Fuels, Lampoldshausen, West Germany, to appear, 1991.

5. E. Gutheil and F.A. Williams, "The Structure of Hydrogen-Air Counterflow Diffusion Flames," Western States Section, The Combustion Institute, Preprint 89-109, Livermore, CA, October, 1989.

6. E. Gutheil and F.A. Williams, "A Numerical and Asymptotic Investigation of Structures of Hydrogen-Air Diffusion Flames at Pressures and Temperatures of High-Speed Combustion," Twenty-Third Symposium (International) on combustion, The Combustion Institute, Pittsburgh, 1991, pp. 513-521.

7. E. Gutheil, G. Balakrishnan and F.A. Williams, "Structure and Extinction of Hydrogen-Air Diffusion Flames", Reduced Kinetic Mechanisms for Applications in Combustion Systems (H. Peters and B. Rogg, editors), Springer-Verlag, to appear, 1991.

8. P.A. Libby, "Comments on the Interaction of Turbulence and Chemical Kinetics," Proceedings of the ICASE/NASA Combustion Workshop, to appear, October 1989.

9. J.S. Kim, P.A. Libby and F.A. Williams, "On the Displacement Effects of Laminar Flames," Western States Section, The Combustion Institute, Boulder, CO, March 19, 1991, and Combustion Science and Technology, submitted, 1991.

10. G. Balakrishnan, A. Liñán and F.A. Williams, "Compressibility Effects in Counterflows," Western States and Canadian Sections, The Combustion Institute, Banff, Alberta, April 29-May 2, 1990.

11. G. Balakrishnan, A. Liñán and F.A. Williams, "Compressibility Effects in Thin Channels with Injection," AIAA Journal, to appear, October 1991.

12. G. Balakrishnan, A. Liñán and F.A. Williams, "Inviscid Flow in Laterally Burning Solid-Propellant Rocket Motors," Western States Section, The Combustion Institute, San Diego, CA, October 14-16,